

## Supplementary Materials

**Table S1:** The protein-protein docking results of HawkDock, ATTRACT and ZDOCK for the 52 newly-added complexes from the ZDOCK Benchmark 4.0.

Target PDB ID	Rank <sup>a</sup>		
	ATTRACT	HawkDock	ZDOCK 3.0.2
1CLV	16	7	1
1F6M	551	790	-
1FCC	12	1562	-
1FFW	7	9	7
1FLE	76	4	334
1GL1	30	28	63
1GXD	175	45	175
1H9D	161	289	41
1HCF	629	192	15
1JIW	1135	6	203
1JK9	41	349	1
1JTG	1974	116	1
1JWH	344	92	14
1JZD	544	512	26
1LFD	173	30	623
1MQ8	71	78	-
1OC0	80	14	364
1OFU	1382	975	746
1OYV	65	110	3
1PVH	1114	1111	1397
1R6Q	114	102	1493
1RV6	1	29	1
1SYX	5	2	117
1US7	277	84	335
1WDW	10	85	6
1XU1	1130	195	7437
1ZHH	234	703	3259
1ZLI	-	-	-
1ZM4	120	7	2
2A5T	4704	290	85
2A9K	962	1074	2626
2ABZ	195	30	248
2AYO	48	115	59
2B4J	1626	3692	5707
2FJU	208	8	393
2G77	698	321	5
2I9B	47	44	261
2IDO	1371	154	20

2J0T	507	3459	60
2J7P	3686	268	-
2O3B	854	141	5296
2OOR	14	6	1285
2OUL	15	1	1
2OZA	22	1	97
2VDB	10	50	100
2Z0E	263	182	205
3BP8	94	50	1573
3CPH	29	6	433
3D5S	18	1	135
3SGQ	5	80	194
4CPA	1	9	1
BOYV	3298	288	-

<sup>a</sup>The rank of the first correct model. “-” means no correct model found.

**Table S2:** The results of the MM/GBSA free energy decomposition.

Target PDB ID <sup>a</sup>	Interface RMSD (Å)	Key residues	Rank <sup>b</sup>		
			Bound structures	Docking models	Top 10 models
1F6M_R (1)	5.750	C138	3	-	/
1FFW_R (2)	1.885	Y106	8	2	4
1GL1_L (3)	1.615	L30	1	1	2
1GXD_R(4)	2.301	K547	7	*	*
		R561	1	*	*
		K617	12	-	/
1H9D_R (5)	2.000	M106	9	7	/
		A107	20	-	/
1HCF_R (6,7)	2.070	R90	6	*	*
		L113	9	3	2
1JIW_L (8,9)	3.435	S2	9	*	*
		L3	7	*	*
		I4	6	*	*
		L5	10	*	*
		A8	-	-	/
1JK9_L (10,11)	2.860	P142	8	-	2
		F36	10	6	/
		H41	-	17	/
		D49	2	-	/
		Y53	14	9	/
		K74	3	2	/
		W112	11	10	/
		F142	1	1	/
		H148	-	-	/
		W150	4	4	4
1JTG_L (12)	2.225	R160	8	7	2
		W162	9	11	/
		E104	11	-	/
		K234	2	-	/
		E240	-	-	/
		R243	4	-	/
		L41	1	3	/
		F54	4	4	/
1JWH_R (17)	2.264	F190	1	1	/
1JZD_R (dimer) (18)	3.657	C118	7	6	/
		C118	16	-	/
1LFD_R (19)	2.203	Y40	1	1	/
1MQ8_L (20)	1.966	L205	1	1	/
		E241	-	11	/

		T243	6	6	/
		E34	-	-	/
		K39	2	3	/
1MQ8_R (21)	1.966	M64	5	4	/
		Y66	3	2	/
		N68	6	5	/
		Q73	4	-	/
1OC0_R (22)	1.274	M110	5	1	/
		Q123	4	8	/
1PVH_R (23)	3.137	D215	9	-	/
		V252	11	-	/
1R6Q_L (24)	2.317	E79	13	3	/
		K84	9	4	/
1RV6_R (25)	1.196	Q27	9	12	/
		D72	6	-	/
		P98	8	6	/
1US7_R (26)	2.419	A107	6	9	/
1XU1_L (27)	2.024	F78	13	12	/
		D80	4	11	/
		L82	1	2	2
		I87	7	3	6
1ZHH_R (28)	3.458	Q23	3	*	*
		V24	4	*	*
		L25	1	*	*
		N26	8	*	*
		Y235	2	5	/
		K254	5	15	/
2A5T_R (29)	2.617	N521	7	2	1
2A5T_L (29)	2.617	E516	3	-	/
2A9K_L (30)	2.543	G99	15	6	/
		E109	-	-	/
2A9K_R (30)	2.543	A103	10	1	/
2B4J_L (31)	3.846	I365	1	1	10
		D366	3	-	/
		F406	5	3	/
		V408	4	4	/
2B4J_R (32)	3.846	V165	-	-	/
		R166	-	-	/
		Q168	9	3	/
		L172	-	-	/
		K173	-	-	/
2FJU_R (33)	1.326	Q52	2	6	/
2FJU_L (33)	1.326	F37	1	6	9
		W56	4	3	3

		L67	5	4	/
		L70	2	2	8
2G77_R (34)	3.878	R343	17	2	/
		Q378	5	-	/
		R490	2	-	/
2I9B_R (35)	5.161	R53	5	-	/
		L55	12	-	/
		Y57	-	-	/
		L66	1	-	/
2I9B_L (36)	5.161	K23	7	8	/
		Y24	2	10	2
2J0T_L (37)	2.045	T2	1	5	/
2O3B_L (38)	4.251	E24	2	20	/
		Q74	-	8	/
		D75	7	-	/
		W76	1	2	2
		T135	13	-	/
2Z0E_L (39)	3.291	F80	4	6	/
		L82	7	-	/
		Q116	3	9	/
		F119	1	1	/
		G120	11	-	/
2Z0E_R (39)	3.291	W142	1	10	/
		R229	7	2	/
3BP8_L (40)	0.965	R424	10	-	2
		V449	3	2	4
		Q456	2	20	8
		A451	5	5	6
3BP8_R (40)	0.965	F136	4	3	/
3D5S_L (41)	1.337	R131	*	4	1
		N138	1	10	8
4CPA_R (42)	1.558	Y248	2	1	1
4CPA_L (43)	1.558	V38	**	2	/

<sup>a</sup>The PDB ID of the complexes reported for the key residues. “R” and “L” represent the receptor and ligand of the protein-protein complex, respectively.

<sup>b</sup>The rank of the key residue. “-” stands for no correct prediction within top 20, “/” stands for no correct prediction within top 10, “\*” stands for no such residue in the structure, and “\*\*” stands for the last residue in the structure with a carboxyl group added by amber and thus cannot be predicted accurately.

### Results

Results for job: example\_rerank **1**

**Downloadable Files:**

- Receptor PDB File
- Ligand PDB File **2**
- HawkDock Output
- Top 10 Predictions
- Top 100 Predictions

**Summary of the top 10 models: 3**

Rank	Residue (Rec)
1	<input type="checkbox"/> A-ILE-164
2	<input type="checkbox"/> A-GLU-37
3	<input type="checkbox"/> A-ASP-163
4	<input type="checkbox"/> A-ALA-101
5	<input type="checkbox"/> A-ASN-98

Showing 1 to 5 of 10 rows  rows per page

< 1 2 >

Rank	Residue (lig)
1	<input type="checkbox"/> B-ARG-27
2	<input type="checkbox"/> B-PHE-38
3	<input type="checkbox"/> B-LEU-35
4	<input type="checkbox"/> B-LEU-55
5	<input type="checkbox"/> B-LYS-31

Showing 1 to 5 of 10 rows  rows per page

< 1 2 >

Rank	Score
1	-28.10
2	-21.68
3	-19.55
4	-18.95
5	-18.53
6	-18.32
7	-14.48
8	-12.80
9	-7.34
10	0.84

### Molecule visualization

**6**

**7**

Model 1  Model 2  Model 3  Model 4  Model 5   
 Model 6  Model 7  Model 8  Model 9  Model 10

**8**

Perform MM/GBSA analysis on top10 model (optional)

Model 1  Model 2  Model 3  Model 4  Model 5   
 Model 6  Model 7  Model 8  Model 9  Model 10

**Submit**

model1	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model1-
model2	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model2-
model3	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model3-
model4	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model4-
model5	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model5-
model6	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model6-
model7	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model7-
model8	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model8-
model9	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model9-
model10	http://cadd.zju.edu.cn/hawkdock/gbsa/example_rerank_model10-

**Action Options: 9**

- **Rotate:** Press and hold the left mouse button.
- **Zoom:** Use mouse's scroll button.
- **Translate:** Press and hold mouse's scroll button.

**Browsers Requirements**

Please make sure that **WebGL** is enabled in your browser. To test for WebGL support, see <http://webglreport.com/?v=1>.

- **Support:** Chrome, Firefox (version 4 or later), Safari, Microsoft Edge, Internet Explorer (version 11).

**Figure S1:** The result page of HawkDock re-ranked by MM/GBSA. At the top left of the page is the job name (1), and under it are the files for downloading (2). The statistics of the 10 most frequency occurring residues for the receptor (3) and ligand (4) are displayed in the table, through which users can specify which residue to show in 3Dmol.js. A summary of the binding free energies for the top 10 models is presented on the left bottom (5). The top 10 models can be viewed in 3Dmol.js (6) with the optional buttons to control which model to display (7). The analysis results of each model are listed under 3Dmol.js (8) and the brief instructions are shown on the bottom (9).

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